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Numerical Latent Heat Observation of the $q = 5$ Potts Model

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The q state Potts model is one of the most intensively studied classical two-dimensional lattice models.[1,2] The model shows second-order phase transition when $q \leq 4$, and shows first-order transition when $q > 4$.[3,2] The critical phenomena of the case $q \leq 4$ have been classified by the conformal field theory.[4,5] Since critical exponents are exactly known for $q = 2, 3$, and 4, the Potts model has been used as a reference system for numerical finite size scaling[6,7] (FSS) analyses. Recently Carlon and Iglói[8] showed that the density matrix renormalization group (DMRG),[9,10,11] which has been applied to classical lattice models,[12,13,14,15] is applicable to the precise estimation of the critical exponents. They also suggest the applicability of DMRG to the first-order phase transition.[8,16]

The phase transition of the two-dimensional $q = 5$ Potts model is often referred as 'weak first-order transition', because the latent heat $L \sim 0.0265$ is especially small compared with the cases $q \geq 6$.[2] To distinguish the weak first-order transition from the second-order transition is a remaining problem in numerical analyses of statistical models, and therefore tow-dimensional $q = 5$ Potts model has been numerically investigated.[17,18,19] At present, it is possible to detect non second-order tendencies in the order parameter[19] or the specific heat.[18] However, quantitative observation of the latent heat L has not been performed. In this short note we calculate the latent heat L of the $q = 5$ Potts model directly by subtracting the site energy of the ordered (= ferromagnetic) phase at the transition temperature from that of the disordered (= paramagnetic) phase. For this purpose we use the corner transfer matrix renormalization group (CTMRG) method.[20,21,22,23]

The outline of CTMRG is as follows. Let us consider a square cluster of q-state Potts model whose linear size is N. The cluster consists of four sub-clusters of the linear size $(N + 1)/2$, which are called as 'corners'.[3] The partition function Z_N is calculated as the trace of $\rho_N = \left(A_{(N+1)/2}\right)^4$, where $A_{(N+1)/2}$ is so called 'corner transfer matrix' (CTM) which transfers column spins into row spins.[3] The point of CTMRG is that ρ_N can be regarded as a kind of density matrix in DMRG, because its trace is the the partition function Z_N. We can therefore apply the renormalization procedure to CTM,[22,23] and transform $A_{(N+1)/2}$ into a renormalized one $\bar{A}_{(N+1)/2}$, which is an m-dimensional matrix. Trace of $\bar{\rho}_N = \left(\bar{A}_{(N+1)/2}\right)^4$ gives a precise lower-bound $\bar{Z}_N$ for the exact partition function Z_N, where the difference $Z_N - \bar{Z}_N$ approaches to zero with increasing m. We can increase the linear size of the corner one by one using a recursive relation between $\bar{A}_n$ and $\bar{A}_{n+1}$, and obtain $\bar{A}_{(N+1)/2}$ for arbitrary N. The renormalized CTM $\bar{A}_{(N+1)/2}$ thus obtained successively gives the approximate partition function $\bar{Z}_N$. In addition to the partition function, we can calculate the site energy and the order parameter at the center of the square cluster.

The partition function of the two-dimensional $q = 5$ Potts model is given by

$$Z^N = \sum_{\{\sigma\}} \exp\left\{ K \sum_{\langle ij \rangle} \delta(\sigma_i, \sigma_j) \right\}, \tag{0.1}$$

where N is the linear dimension of the finite size system, σ_i is the five-state spin variable on the lattice point i, $\langle ij \rangle$ specifies the neighboring spin pairs, and $\delta(\sigma_i, \sigma_j)$ is equal to unity only when $\sigma_i = \sigma_j$ and zero otherwise. We consider both paramagnetic boundary conditions (PBC), where arbitrary spin configurations are allowed at the boundary, and ferromagnetic boundary conditions (FBC), where boundary spins are fixed to the same direction. In the limit of $N \to \infty$, the $q = 5$ Potts model shows first-order phase transition when the parameter K is equal to

$$K_c = \ln\left(\sqrt{5} + 1\right). \tag{0.2}$$

At the transition point, the site energy

$$U = 2\langle \delta(\sigma_i, \sigma_j) \rangle \tag{0.3}$$

of the disordered (= high-temperature) phase U^+ differs from that of the ordered (= low-temperature) phase U^- by the latent heat $L \sim 0.0256$. The average of U^+ and U^- is simply expressed as $U_0 = 1/2 + 1/2\sqrt{5}$, that is obtained by the duality relation.[3,2]

In order to estimate $U^\pm$ numerically, we first calculate the site energy $U_N^+(m)$ and $U_N^-(m)$ at the center of square cluster of size N, respectively, by imposing PBC and FBC when $K = K_c$. The number m is the matrix dimension of the renormalized CTM $\bar{A}_{(N+1)/2}$. It should be noted that $U^\pm$ is equal to $\lim_{m\to\infty}\lim_{N\to\infty} U_N^\pm(m)$. Figure 1 shows $U_N^\pm(m)$ for $m = 40, 67$ and 200 up to

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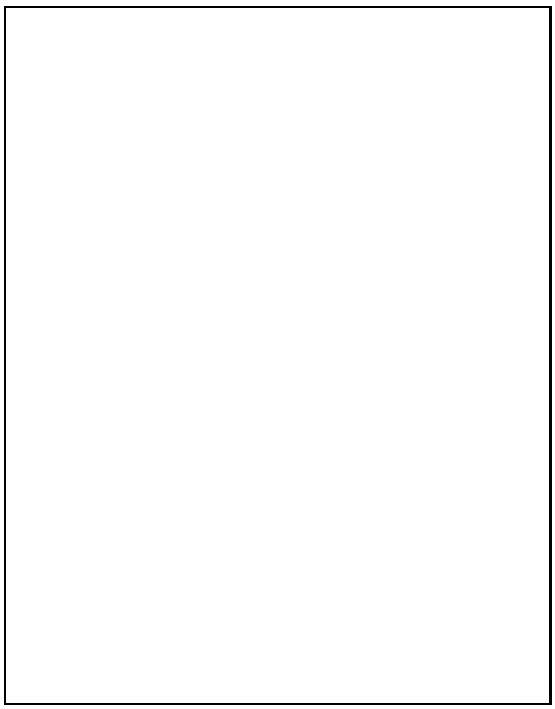

Fig. 1. System size dependence of the site energy for both fixed and free boundary conditions.

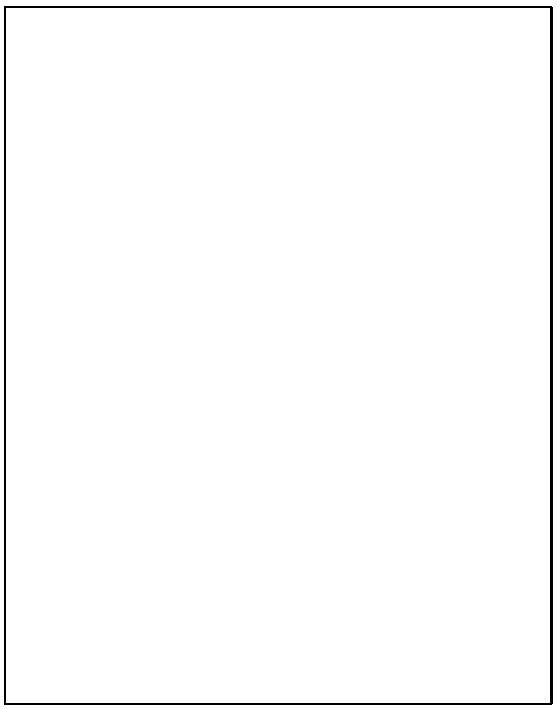

Fig. 2. The m dependence of $U_\infty^\pm(m)$. The $1/m$ extrapolation gives the latent heat L.

$N = 4000$. We choose U_0 as the zero of the site energy. The m dependence of $U_N^\pm(m)$ is not negligible in the large N region, where the energy $U_N^\pm(m)$ approaches to $U_\infty^\pm(m)$ exponentially with respect to N.

Figure 2 shows the m dependence of $U_\infty^\pm(m)$. There is m dependence because the energy cut-off introduced by the renormalization group transformation is comparable to the latent heat L. As shown in Fig.2, $U_\infty^\pm(m)$ is nearly linear in $1/m$, and therefore we may linearly extrapolate $U_\infty^\pm(m)$ to obtain $U^\pm = U_\infty^\pm(\infty)$. As a result we obtain $U^+ = U_0 - 0.014$ and $U^- = U_0 + 0.013$, where the obtained U^+ and U^- are slightly lower than the exact ones. We finally obtain the latent heat $L = U^- - U^+ = 0.027$, which quantitatively agrees with the exact one $L \sim 0.0265$. As far as we know, this is the first quantitative estimate of the latent heat by numerical calculation.

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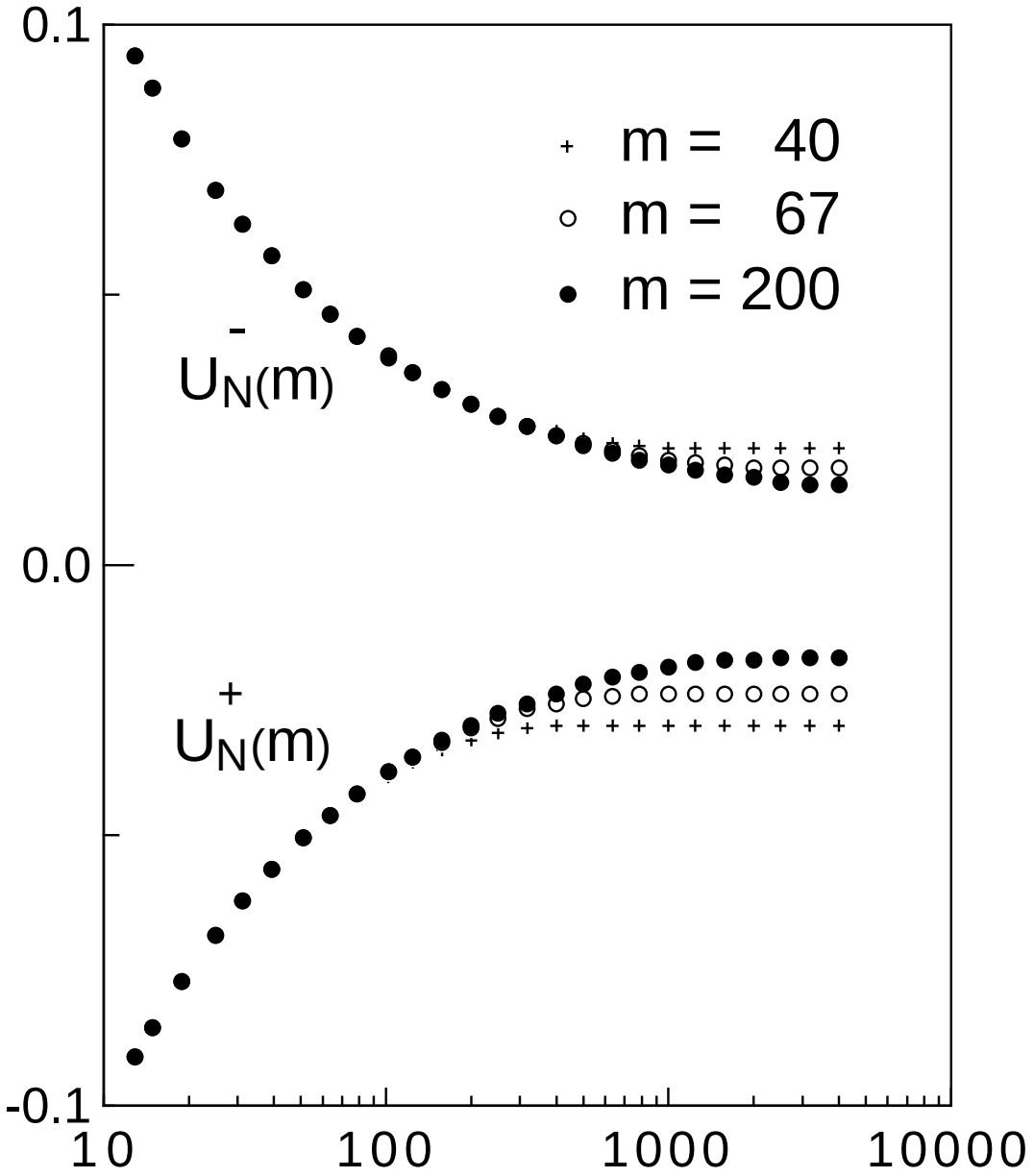

Fig. 1.
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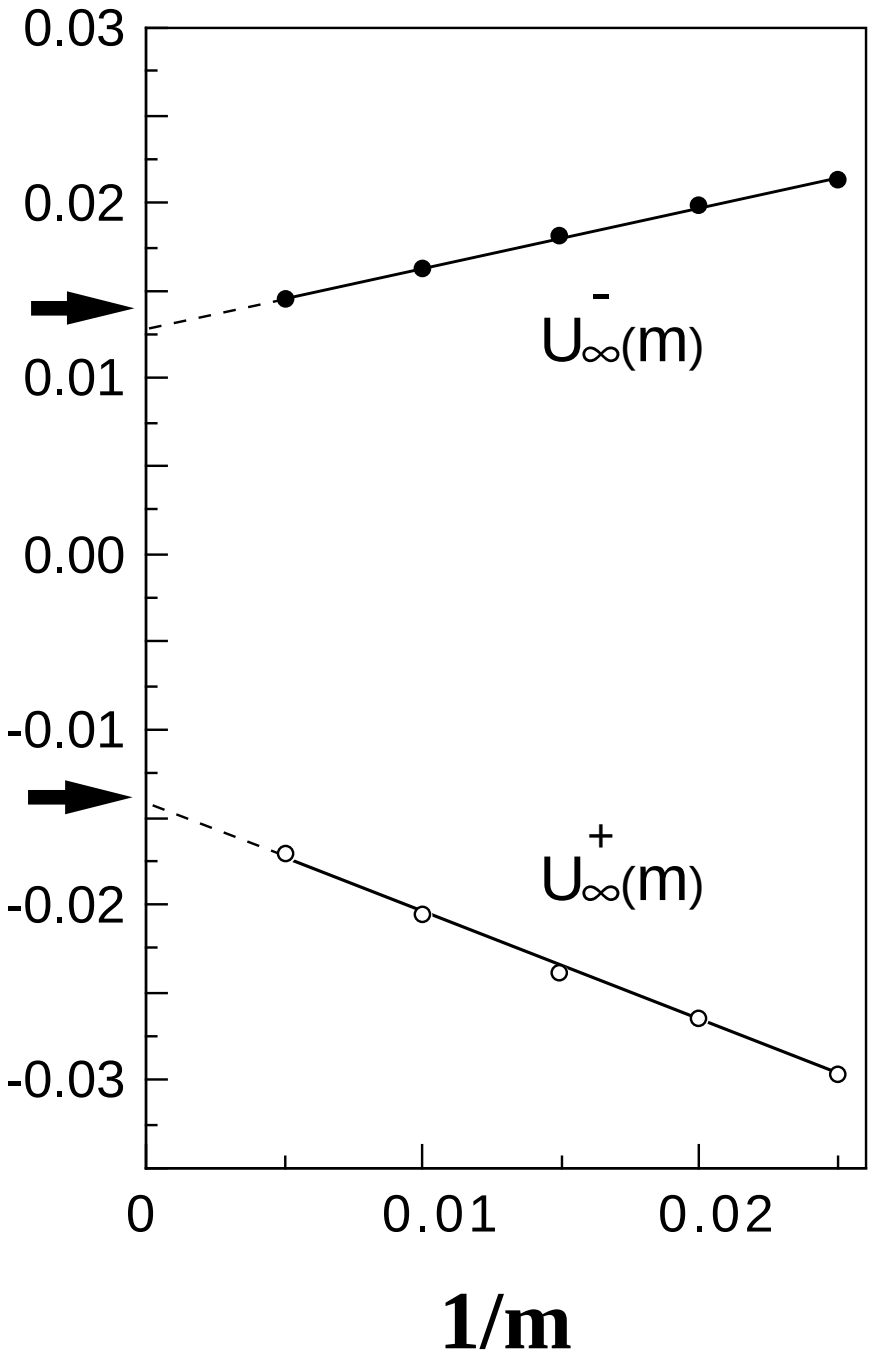

Fig. 2.
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